

An implicit rheological model for numerical simulation of generalized Newtonian fluids

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Fitting an explicit curve over some discrete data extracted from a rheometer is the usual way of writing a rheological model for generalized Newtonian fluids. These explicit models may not match totally with the extracted data and may ignore some features of the rheological behavior of the fluids. In this paper, a cubic-spline curve fitting is used to fit a smooth curve from discrete rheological data. Spline interpolation avoids the problem of Runge's phenomenon, which occurs in interpolating using high degree polynomials. The formulation for applying presented rheological model is described in the context of least squares meshfree technique. One problem is solved to show validity of the scheme: a fluid with rather complex rheology model is considered and solved by both conventional explicit and proposed implicit models to show the advantages of the presented method.

Keywords: cubic spline, collocated discrete least squares, meshless method, radial point interpolation

1. Introduction

The relation between the rate of the strain and apparent viscosity shows the basic characteristic of the deformation behavior of a generalized Newtonian fluid. There are some well known models which are used to describe the mentioned relation explicitly. In the power-law model (Blair *et al.*, 1939), the apparent viscosity varies as a power of strain rate. This model can be used to simulate both shear thinning and shear thickening behavior of a fluid by tuning its parameter. When there are significant deviations from the power-law model at very high and very low shear rates, it is necessary to use a model which takes account of the limiting values of viscosities. Based on the molecular network considerations, Carreau (1972) presented a rheology model which limits the value of the apparent viscosity at extreme values of shear rate (or rate of strain). Cross (1965) presented a four-parameter model, which also considers limiting values for the viscosity at low and high values of the shear rates. The Bingham plastic model (Bingham, 1916) is the simplest equation, which describes the flow of a fluid with a yield stress. Herschel–Bulkley model by Herschel and Bulkley (1926) uses a three constant explicit equation to describe the nonlinearity of a fluid with plastic behavior. Casson model was used by Blair (1959) to describe the rheological behavior of many fluids in food industry, blood and biological fluids. Comprehensive reviews on rheological models were presented by Bird (1987) and Macosko (1994).

All of the mentioned models use an explicit formulation with some adjustable parameters to fit an appropriate

curve over some scattered given data. In this paper, an implicit cubic-spline method is used to fit a curve over the shear rate-apparent viscosity data. Spline interpolation avoids the problem of Runge's phenomenon. The problem of oscillatory results of interpolation with polynomials of high degree, near the ends of an interval, calls Runge's phenomenon.

In the present study, this implicit model is linked to the governing equations to be used in the calculation of the viscosity and its derivatives at any point in the domain of a problem. A least squares based meshfree method named collocated discrete least squares (CDLS) is used in the numerical solution of the problems. The method presented by Afshar and Lashkarbolok (2008) is integral free, simple in formulation, and flexible in domain discretization. Here, the governing equations are considered to be solved implicitly. It means that the evolution of the pressure, velocity and stresses are computed simultaneously at each time step. To connect the pressure to the continuity equation, conventional artificial compressibility technique is used. The presented rheology model is limited to isothermal problems but with some modifications, it can consider the temperature effect on the viscosity. In this case, two dimensional version of cubic spline may be used to obtain required viscosity at given shear rate and temperature at any point in the domain of the problem. In addition, energy equation must be added to the governing equations to find the temperature distribution at any point in the fluid. In this paper, we focus on the isothermal problems.

Although the problems are assumed to be steady state, the governing equations are solved in time to the point that a steady-state solution is obtained. To validate the proposed method, a benchmark problem of cavity flow

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with non-Newtonian fluid is considered. Bell and Surana (1995) solved this problem using a power-law model. Here, the problem is solved in the same condition by using the proposed implicit model instead of explicit power-law model. To show the priority of the proposed scheme over conventional methods, a fluid with rather complicated rheology is considered. Aqueous solutions of urethane-coupled poly(ethylene oxide) show both shear thinning and shear thickening behaviors (Yekta *et al.*, 1995). In the second problem, this fluid is put into the cavity and the problem is solved by using the proposed implicit model.

2. Governing Equations and Implicit Rheological Model

Governing equations comprise of continuity, momentum, and constitutive equations for two dimensional incompressible flow of a generalized Newtonian fluid. They are given in Cartesian coordinates as

$$\frac{\partial u^*}{\partial t^*} + u^* \frac{\partial u^*}{\partial x^*} + v^* \frac{\partial u^*}{\partial y^*} = -\frac{1}{\rho_0} \frac{\partial p^*}{\partial x^*} + \frac{1}{\rho_0} \left(\frac{\partial \tau_{xx}^*}{\partial x^*} + \frac{\partial \tau_{xy}^*}{\partial y^*} \right), \quad (1)$$

$$\frac{\partial v^*}{\partial t^*} + u^* \frac{\partial v^*}{\partial x^*} + v^* \frac{\partial v^*}{\partial y^*} = -\frac{1}{\rho_0} \frac{\partial p^*}{\partial y^*} + \frac{1}{\rho_0} \left(\frac{\partial \tau_{yx}^*}{\partial x^*} + \frac{\partial \tau_{yy}^*}{\partial y^*} \right), \quad (2)$$

$$\frac{\partial u^*}{\partial x^*} + \frac{\partial v^*}{\partial y^*} = 0, \quad (3)$$

$$\tau_{xx}^* = 2\eta^* \frac{\partial u^*}{\partial x^*}, \quad (4)$$

$$\tau_{xy}^* = \tau_{yx}^* = \eta^* \left(\frac{\partial u^*}{\partial y^*} + \frac{\partial v^*}{\partial x^*} \right), \quad (5)$$

$$\tau_{yy}^* = 2\eta^* \frac{\partial v^*}{\partial y^*} \quad (6)$$

where u^* , v^* , and p^* are velocity component in x direction, velocity component in y direction, and pressure, respectively. η^* is the apparent viscosity that depends on the magnitude of strain rate in isothermal condition. The magnitude of strain rate is defined by the second invariant of its tensor that will be shown by $|\dot{\gamma}|^*$. It is defined as

$$|\dot{\gamma}|^* = \sqrt{2\left(\frac{\partial u^*}{\partial x^*}\right)^2 + 2\left(\frac{\partial v^*}{\partial y^*}\right)^2 + \left(\frac{\partial u^*}{\partial y^*} + \frac{\partial v^*}{\partial x^*}\right)^2}. \quad (7)$$

To illustrate the proposed rheology model, assume a tabulated values of the apparent viscosity (η^*) versus $|\dot{\gamma}|^*$, which is given in Table 1. These data are belonging to an aqueous solution of urethane-coupled polymers containing $C_{16}H_{33}O$ end groups, which is taken from the research of Yekta *et al.* (1995). This fluid shows both shear thinning and shear thickening behavior. Since there is a wide range

Table 1. Values of viscosity at different shear rates $|\dot{\gamma}|^*$ (1/s) for AT 22-3 (Yekta *et al.*, 1995).

$\log \dot{\gamma} ^*$ (1/s)	η^* (Pa.s)
-0.42313	3.119691
-0.21174	3.196911
-0.00107	3.150579
0.198057	3.135135
0.386734	3.335907
0.586586	3.444015
0.786981	3.644788
0.98801	3.953668
1.189129	4.277992
1.388257	4.262548
1.607837	3.737452
1.801173	2.733591
2.007043	1.868726
2.200018	0.803089
2.396522	0.339768
2.595017	0.216216

in the values of $|\dot{\gamma}|^*$, it is advisable to use a logarithmic scale to make a better quality interpolation. Here, a cubic spline (c-spline) method is used to find an approximate value of the apparent viscosity at any value of $|\dot{\gamma}|^*$. For Table 1, the approximate values of the apparent viscosity at other points are calculated by c-spline method, as shown in Fig. 1. To make a comparison between c-spline and explicit models, three explicit models (i.e., power-law, Carreau-Yasuda, and Cross) are used to fit curves over the given rheology data in Table 1. The results of these

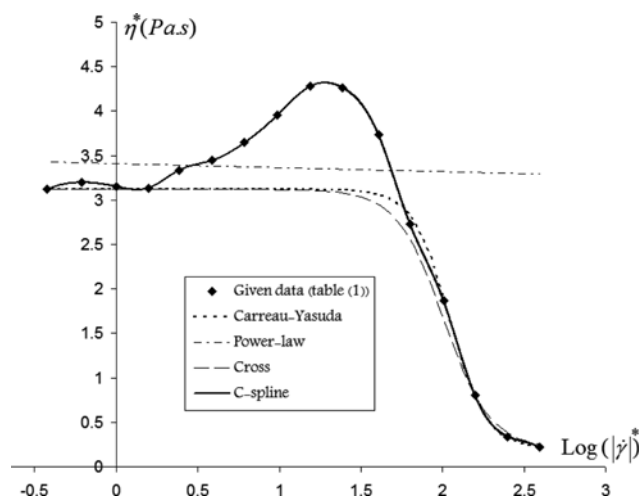


Fig. 1. Approximate values of η^* using c-spline and three explicit models for given data in Table 1.

explicit models are also shown in Fig. 1. Although the chosen parameters of explicit models in the curve fitting procedure might be not completely optimized, according to Fig. 1, we can claim that they cannot reach to the accuracy of c-spline method in this problem. C-spline gives a smooth and differentiable curve in which passes through all rheology data without facing with Runge's phenomenon.

It is required to find the derivative values of apparent viscosity with respect to x^* and y^* in Eqs. (1) and (2). These derivatives are calculated by using a chain rule, given by

$$\frac{\partial \eta^*}{\partial x^*} = \frac{d\eta^*}{d|\dot{\gamma}^*|} \frac{\partial |\dot{\gamma}^*|}{\partial x^*} = \frac{d\eta^*}{d(\log|\dot{\gamma}^*|)} \frac{1}{|\dot{\gamma}^*| \ln(10)} \frac{\partial |\dot{\gamma}^*|}{\partial x^*}, \quad (8)$$

$$\frac{\partial \eta^*}{\partial y^*} = \frac{d\eta^*}{d|\dot{\gamma}^*|} \frac{\partial |\dot{\gamma}^*|}{\partial y^*} = \frac{d\eta^*}{d(\log|\dot{\gamma}^*|)} \frac{1}{|\dot{\gamma}^*| \ln(10)} \frac{\partial |\dot{\gamma}^*|}{\partial y^*}, \quad (9)$$

$$\frac{\partial |\dot{\gamma}^*|}{\partial x^*} = \frac{1}{2} \frac{\left[4 \frac{\partial^2 u^*}{\partial x^{*2}} \left(\frac{\partial u^*}{\partial x^*} - \frac{\partial v^*}{\partial y^*} \right) + 2 \left(\frac{\partial^2 v^*}{\partial x^{*2}} - \frac{\partial^2 v^*}{\partial y^{*2}} \right) \left(\frac{\partial u^*}{\partial y^*} + \frac{\partial v^*}{\partial x^*} \right) \right]}{\left[2 \left(\frac{\partial u^*}{\partial x^*} \right)^2 + 2 \left(\frac{\partial v^*}{\partial y^*} \right)^2 + \left(\frac{\partial u^*}{\partial y^*} + \frac{\partial v^*}{\partial x^*} \right)^2 \right]^{1/2}}, \quad (10)$$

$$\frac{\partial |\dot{\gamma}^*|}{\partial y^*} = \frac{1}{2} \frac{\left[4 \frac{\partial^2 v^*}{\partial y^{*2}} \left(\frac{\partial v^*}{\partial y^*} - \frac{\partial u^*}{\partial x^*} \right) + 2 \left(\frac{\partial^2 u^*}{\partial y^{*2}} - \frac{\partial^2 u^*}{\partial x^{*2}} \right) \left(\frac{\partial u^*}{\partial y^*} + \frac{\partial v^*}{\partial x^*} \right) \right]}{\left[2 \left(\frac{\partial u^*}{\partial x^*} \right)^2 + 2 \left(\frac{\partial v^*}{\partial y^*} \right)^2 + \left(\frac{\partial u^*}{\partial y^*} + \frac{\partial v^*}{\partial x^*} \right)^2 \right]^{1/2}}. \quad (11)$$

3. Collocated Discrete Least Squares (CDLS) Formulations

To obtain an evolution equation for the pressure in the numerical solution of Eqs. (1)-(3), a pseudo time derivative of the pressure is added to the continuity equation. Chorin (1967) introduced this method of artificial compressibility. A parameter C is introduced that is referred to the artificial speed of sound. The value of C is usually chosen to be near the value of characteristic velocity (Rogers *et al.*, 1987). The time dependent forms of the dimensionless governing equations are given by

$$\begin{aligned} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \\ - \frac{\partial p}{\partial x} + \frac{1}{Re} \left[2 \frac{\partial \eta}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial \eta}{\partial y} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \eta \left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial x^2} \right) \right], \end{aligned} \quad (12)$$

$$\begin{aligned} \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = \\ - \frac{1}{\rho} \frac{\partial p}{\partial y} + \frac{1}{Re} \left[2 \frac{\partial \eta}{\partial y} \frac{\partial v}{\partial y} + \frac{\partial \eta}{\partial x} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \eta \left(\frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial x^2} \right) \right], \end{aligned} \quad (13)$$

$$\frac{\partial p}{\partial t} + C \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) = 0. \quad (14)$$

Eqs. (12)-(14) are written by considering the followings: $u = u^*/u_0$, $v = v^*/u_0$, $t = t^*u_0/L_0$, $x = x^*/L_0$, $y = y^*/L_0$, $p = p^*/\rho_0 u_0^2$, and $\eta = \eta^*/\eta_{ref}$. Here, $Re = \rho_0 u_0 L_0 / \eta_{ref}$ is the Reynolds number, where ρ_0 , u_0 , L_0 , and η_{ref} are characteristic density, velocity, length, and reference viscosity, respectively.

Eqs. (12)-(14) are solved in time to the point that a steady state solution is obtained. For the temporal discretization, the first order accurate implicit Euler method is used, given by

$$\begin{aligned} \frac{u^{t+1} - u^t}{\Delta t} + u^t \frac{\partial u^{t+1}}{\partial x} + v^t \frac{\partial u^{t+1}}{\partial y} = - \frac{\partial p^{t+1}}{\partial x} + \\ \frac{1}{Re} \left[2 \frac{\partial \eta^t}{\partial x} \frac{\partial u^{t+1}}{\partial x} + \frac{\partial \eta^t}{\partial y} \left(\frac{\partial u^{t+1}}{\partial y} + \frac{\partial v^{t+1}}{\partial x} \right) + \eta^t \left(\frac{\partial^2 u^{t+1}}{\partial y^2} + \frac{\partial^2 u^{t+1}}{\partial x^2} \right) \right], \end{aligned} \quad (15)$$

$$\begin{aligned} \frac{v^{t+1} - v^t}{\Delta t} + u^t \frac{\partial v^{t+1}}{\partial x} + v^t \frac{\partial v^{t+1}}{\partial y} = - \frac{\partial p^{t+1}}{\partial y} + \\ \frac{1}{Re} \left[2 \frac{\partial \eta^t}{\partial y} \frac{\partial v^{t+1}}{\partial y} + \frac{\partial \eta^t}{\partial x} \left(\frac{\partial u^{t+1}}{\partial y} + \frac{\partial v^{t+1}}{\partial x} \right) + \eta^t \left(\frac{\partial^2 v^{t+1}}{\partial y^2} + \frac{\partial^2 v^{t+1}}{\partial x^2} \right) \right], \end{aligned} \quad (16)$$

$$\frac{p^{t+1} - p^t}{\Delta t} + C \left(\frac{\partial u^{t+1}}{\partial x} + \frac{\partial v^{t+1}}{\partial y} \right) = 0 \quad (17)$$

where t and $t+1$ are previous and next time steps, respectively. The idea of the least squares method is to find a solution minimizing the residuals arising from the approximation. The mathematical basis of the CDLS method is described in detailed in the previous papers (e.g. Lashkarbolok and Jabbari, 2012; Lashkarbolok and Jabbari, 2013; Lashkarbolok *et al.*, 2014). In this section, the formulation of the method for solving the governing equations is subsequently illustrated in a simple matrix format.

Step 1. Domain discretization

Domain of the problem must be discretized by two set of scatter nodes. They named field and collocation points. Results will be calculated in the field nodes and it can be interpolated to the collocation points. Collocation points will not change the size of the final coefficient matrix and help the method to obtain better results (Afshar and Lashkarbolok, 2008). The approximate value of the function ϕ at a collocation point k with the coordinate of (x_k, y_k) can be obtained through the following interpolation: $\phi(x_k, y_k) = \sum_{i=1}^{\bar{n}} N_i(x_k, y_k) \phi_i$, where ϕ_i is the value of the unknown function at i -th field node. \bar{n} is the number of field nodes at k -th collocation point in its domain. $N_i(x_k, y_k)$ is the value of the shape function of i -th node at k -th collocation point.

Step 2. Shape function calculation

Function approximation is the base of numerical method. In the present study, radial point interpolation method (RPIM) is used in function approximation. Detailed

description of the procedure is available in the literature (Liu, 2002). Throughout this paper, a multi quadratic radial basis function augmented with polynomials of completed second order is applied in the RPIM. The multi quadratic radial basis function (q) used in this paper is given by

$$q(r) = (ds^2 + r^2)^{3.5} \tag{18}$$

where r is the Euclidian distance between a field and collocation point. For the problems solved here, ds is the radius of the compact support domain, and the number of nodes to support collocation points is defined by \bar{n} (cf. Here, it is consider 25). Then, for each collocation, a radius (ds) is determined so that \bar{n} nodes place in the domain of that point. To write a matrix formulation, we should put the values of the shape functions and their derivatives into some matrices. If domain of the problem is discretized using n_p nodes and n_c collocation points, the size of shape function matrix (N) and its derivatives (i.e., $\partial N/\partial x$, $\partial^2 N/\partial x^2$, $\partial N/\partial y$, and $\partial^2 N/\partial y^2$) must be $n_p \times n_c$. Since a compact support domain is used, there are a few non-zero elements in each row of those matrices so that they can be considered as sparse matrices and may be saved efficiently in the memory of computer (Lashkarbolok *et al.*, 2014).

Step 3. Finding coefficients and right hand side matrices

A simple pattern is proposed to write the coefficient and right hand side vector. Here, Eqs. (15)-(17) considered to be solved simultaneously as system of partial differential equations (cf. 3 equations with 3 unknowns). Let us consider Eq. (15). To write the first array (Lb_{11}) of the coefficient matrix (cf. it is a matrix itself), we replace the variable u^{t+1} by the matrix N , meaning that

$$Lb_{11} = N + \Delta t \left[u' \otimes \frac{\partial N}{\partial x} + v' \otimes \frac{\partial N}{\partial y} - \frac{1}{Re} \left(2 \frac{\partial \eta'}{\partial x} \otimes \frac{\partial N}{\partial x} + \frac{\partial \eta'}{\partial y} \otimes \frac{\partial N}{\partial y} \right) + \eta' \otimes \left(\frac{\partial^2 N}{\partial y^2} + \frac{\partial^2 N}{\partial x^2} \right) \right]. \tag{19}$$

Here, the operator \otimes is defined by Lashkarbolok *et al.* (2015). Similarly, Lb_{12} can be calculated by replacing v^{t+1} in Eq. (15) by the matrix N , given as

$$Lb_{12} = -\frac{\Delta t}{Re} \frac{\partial \eta'}{\partial y} \otimes \frac{\partial N}{\partial x}. \tag{20}$$

The remained arrays are calculated in the same way, then the coefficient matrix (K) and right hand side vector (F) can be written by

$$L = \begin{bmatrix} Lb_{11} & Lb_{21} & Lb_{31} \\ Lb_{12} & Lb_{22} & Lb_{32} \\ Lb_{13} & Lb_{23} & Lb_{33} \end{bmatrix}, \tag{21}$$

$$K = L L^T, \tag{22}$$

$$F = L \begin{bmatrix} u' \\ v' \\ p' \end{bmatrix}. \tag{23}$$

It should be noted that, since the shape function matrices are sparse, all matrix operations can be performed efficiently. The values of u , v , and p (all in a vector U) at $(t+1)$ -th time step can be found by

$$U^{t+1} = K/F. \tag{24}$$

The symmetry and positive definiteness of K make it suitable for the efficient iterative solvers.

4. Numerical Examples

In this section, the lid driven cavity flow problem is solved with two different types of fluids. The geometry and boundary conditions of the problem are shown in Fig. 2.

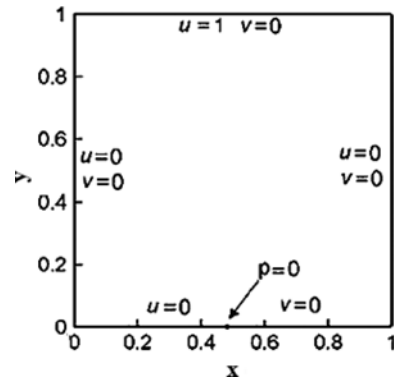


Fig. 2. Geometry and boundary condition in lid-driven cavity flow problem (Firoozjaee and Afshar, 2010).

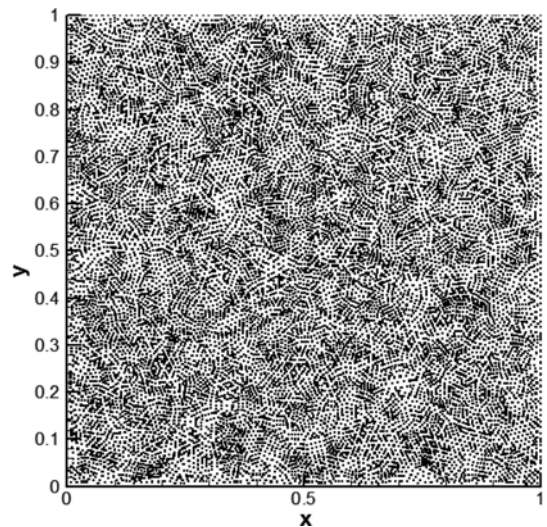


Fig. 3. The position of field nodes in domain discretization.

In the solution of the following problems, Δt and C are chosen to be 0.1 s and 1, respectively. In the first problem, the proposed method is used to solve a power law fluid. Instead of using an explicit model in the governing equations, the proposed implicit model is used to solve the problem. After that, the cavity flow problem is solved using more complex rheological data. In domain discretization, 15,863 nodes along with 34,988 collocation points, which distributed irregularly in the domain of the problem, are used for both problems. The position of field nodes is shown in Fig. 3.

Problem 1:

The proposed scheme is applied to solve a fluid flow with some discrete rheological data which are given in Table 2. These data are perfectly matched with a power-law fluid with the explicit formulation of $\eta^* = |\dot{\gamma}^*|^{-0.5}$. Bell and Surana (1995) solved this problem at some Reynolds numbers using explicit power-law model. Here, instead of using the explicit formulation, the problem is solved by the presented implicit method using discrete data given in Table 2.

To make a comparison with the results of Bell and Surana (1995), the parameters are chosen as $u_0 = 1$ m/s, $L_0 = 1$ m, $\eta_{ref} = 1$ Pa·s, and $Re = 100$. The contours of apparent viscosity η and streamlines are shown in Figs. 4 and 5. In Fig. 6, the mid span profile of the horizontal velocity is calculated and compared with the results of Bell and Surana (1995). Results show a good agreement with the previous study performed by explicit model.

Problem 2:

Assume the values of the viscosity at some shear rates

Table 2. Values of viscosity at different shear rates $|\dot{\gamma}^*|$ (1/s) for Problem 1.

$\log \dot{\gamma}^* $ (1/s)	η^* (Pa·s)
-3	31.622777
-2.5	17.782794
-2	10
-1.5	5.6234133
-1	3.1622777
-0.5	1.7782794
0	1
0.5	0.5623413
1	0.3162278
1.5	0.1778279
2	0.1
2.5	0.0562341
3	0.0316228

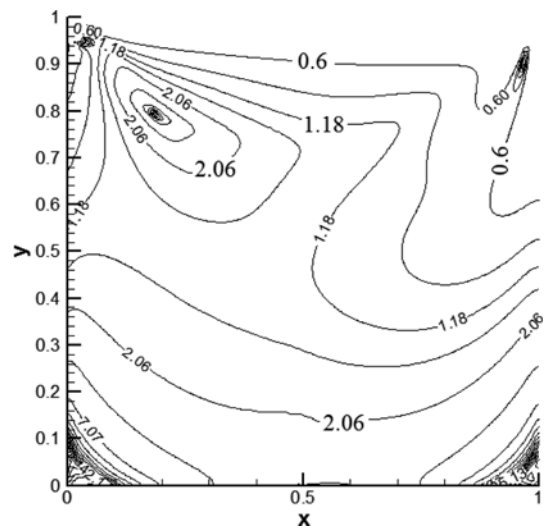


Fig. 4. Apparent viscosity contours for Problem 1.

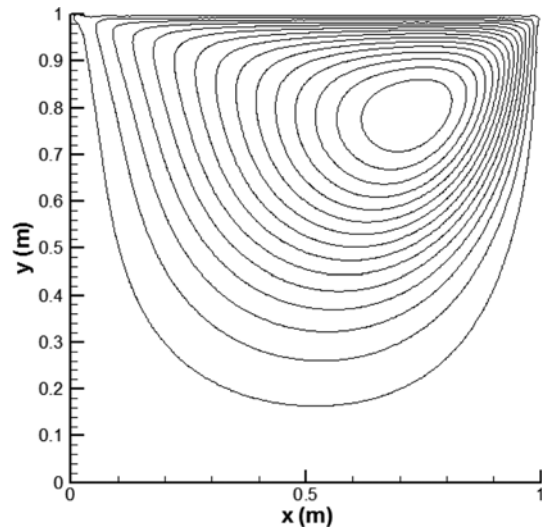


Fig. 5. Stream lines for Problem 1.

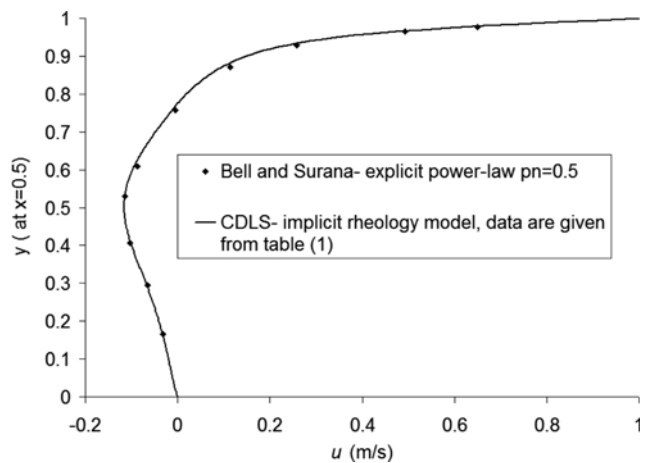


Fig. 6. Mid span profile of horizontal velocity u at $x = 0.5$.

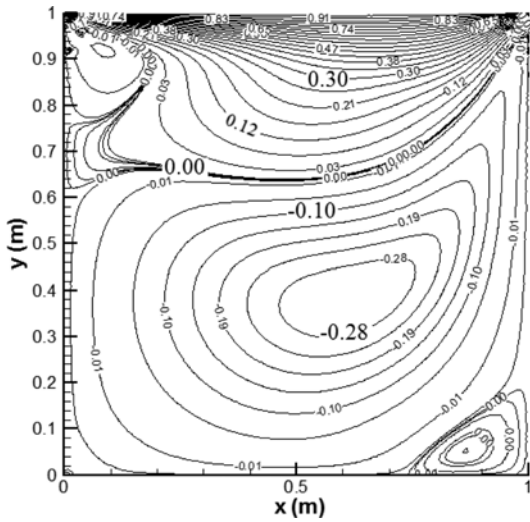


Fig. 7. Horizontal velocity contours for Problem 2.

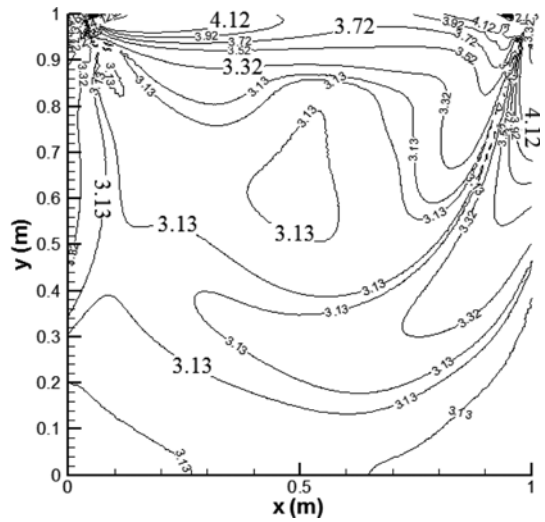


Fig. 9. Apparent viscosity (η^*) contours for Problem 2.

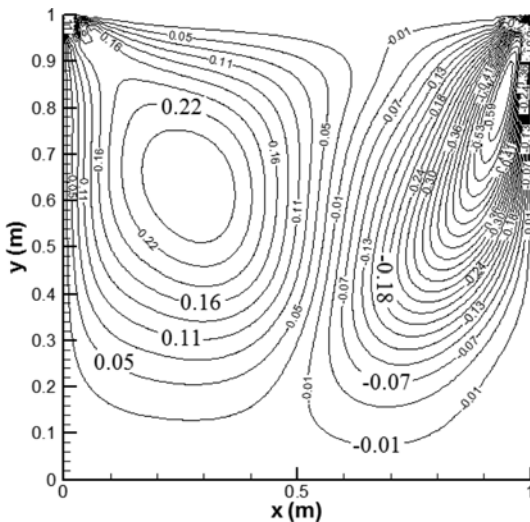


Fig. 8. Vertical velocity contours for Problem 2.

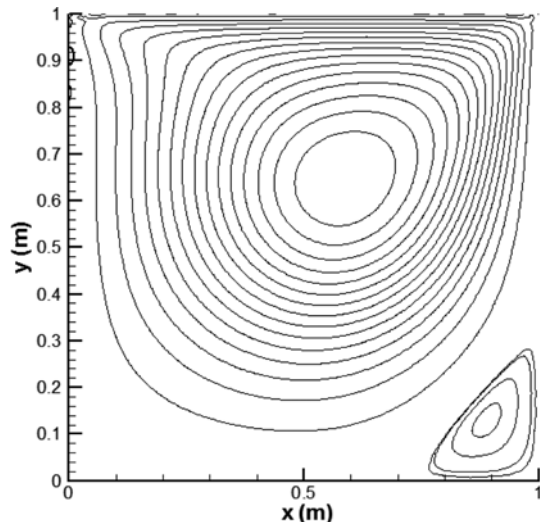


Fig. 10. Streamlines for Problem 2.

are given in Table 1. The approximate values of the viscosity at required shear rates are calculated by c-spline method, as shown in Fig. 1. For this problem, parameters are chosen as: $u_0 = 1$ m/s, $L_0 = 1$ m, $\eta_{ref} = 0.2$ Pa·s, and $Re = 5000$. This fluid is put in the defined cavity problem and solved using proposed scheme. The horizontal velocity, vertical velocity, and viscosity contours are shown in Figs. 7-9, and streamlines are shown in Fig. 10.

5. Conclusions

An implicit rheological model based on a spline function approximation was presented. The methodology is linked with a meshfree technique to solve the equations of motion for the generalized Newtonian fluids. The proposed scheme is suitable to simulate the flow of viscous

fluids with complex rheological behavior as well as fluids with simple rheological models. The fitted curve passes through all rheology data smoothly. A fully matrix formulation was presented to make the procedure easy to code and efficient in calculation, and this method was validated by solving a benchmark problem. The results show a good agreement with the literature. Then, the fluid flow with a complex rheology was dealt with to show the priority of the proposed implicit model over explicit models in fitting a differentiable curve over rheology data.

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